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Electronic properties of LaAlO3/SrTiO3n-type interfaces: A GGA+U study

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Abstract

© 2017 IOP Publishing Ltd. Printed in the UK. LaAlO 3 /SrTiO 3 heterostructures as covered by the on-site Coulomb repulsion within the GGA U approach is investigated. Performing a systematic variation of the values of the Coulomb parameters applied to the Ti 3d and La 4f orbitals we put previous suggestions to include a large value for the La 4f states into perspective. Furthermore, our calculations provide deeper insight into the band gap landscape in the space spanned by these Coulomb parameters and the resulting complex interference effects. In addition, we identify important correlations between the local Coulomb interaction within the La 4f shell, the band gap, and the atomic displacements at the interface. In particular, these on-site Coulomb interactions influence buckling within the LaO interface layer, which via its strong coupling to the electrostatic potential in the LAO overlayer causes considerable shifts of the electronic states at the surface and eventually controls the band gap.

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Keywords

electronic structure, GGA+U, LAO/STO heterostructure

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